

# On the unitarity of S-matrix in 1-d case

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It is shown that the scattering S-matrix is unitary even if the scattering potential  $U(x)$  tends to different limits at  $x \rightarrow \pm\infty$ . This result is in contrast to the statements of some authors which argue that the unitarity may be broken in 1-d case if  $U(-\infty) \neq U(+\infty)$ . The mistake may result from a wrong normalization of the wave functions. This work may be considered as a comment to some of those works.

A fundamental property of the scattering S-matrix is its unitarity (c.f. e.g. Ref.[1]). This is a consequence of the particle conservation law. However, there have appeared a number of works<sup>2-5</sup> where the S-matrix obtained or used is not unitary, and the authors have accepted this as a special feature of the problem owing to the different behavior of the potential at  $\pm\infty$ . This work may be considered as a comment on those works. It consists of two parts. First, we repeat a wrong derivation using a simple example and then prove the unitarity of the scattering matrix in the general case.

Let us consider a step potential of the form:

$$U(x) = \begin{cases} 0, & x < 0 \\ U_0, & x > 0 \end{cases} \quad (1)$$

The general solution of the Schrödinger equation is well known:

$$\begin{aligned} \psi_l &= Ae^{ikx} + Be^{-ikx}, & x < 0 \\ \psi_r &= Ce^{i\kappa x} + De^{-\kappa x}, & x > 0 \end{aligned} \quad (2)$$

where  $k = \sqrt{2E}$ ,  $\kappa = \sqrt{2(E - U_0)}$  and for simplicity we put  $\hbar = m = 1$ . Let us consider the most instructive case when  $E > U_0$ . The constants  $A, B, C, D$  have to satisfy the relations  $\psi_l(0) = \psi_r(0)$  and  $\psi'_l(0) = \psi'_r(0)$ . This yields

$$A + B = C + D, \quad k(A - B) = \kappa(C - D) \quad (3)$$

The S-matrix components connect the incoming waves ( $Ae^{ikx}$  and  $De^{-\kappa x}$ ) with the outgoing ones ( $Be^{-ikx}$  and  $Ce^{i\kappa x}$ ). If one defines the S-matrix by the relation

$$\begin{pmatrix} A \\ D \end{pmatrix} = \tilde{S} \begin{pmatrix} C \\ B \end{pmatrix} \quad (4)$$

it will be of the form

$$\tilde{S}_{11} = \frac{2\kappa}{k + \kappa}, \quad \tilde{S}_{22} = \frac{2k}{k + \kappa}, \quad \tilde{S}_{12} = -\tilde{S}_{21} = \frac{k - \kappa}{k + \kappa} \quad (5)$$

The quantity  $R = \tilde{S}_{12}^2 = \tilde{S}_{21}^2$  coincides with the reflection coefficient, but  $\tilde{S}_{11}$  and  $\tilde{S}_{22}$  have no physical meaning. They are not transmission amplitudes, at least because  $\tilde{S}_{11}^2 + \tilde{S}_{12}^2 \neq 1$ . Therefore,  $\tilde{S}$  is not the scattering matrix of our problem.

Let us now derive the correct form of the S-matrix. We shall do this for an arbitrary potential of the form:

$$U(x \rightarrow -\infty) = 0, \quad U(x \rightarrow \infty) = U_0 \quad (6)$$

Therefore, the asymptotes at  $\pm\infty$  are of the form (2). However, for calculating the scattering S-matrix components *these functions have to be normalized to unit flux, not to unit density!* Only in this case the S-matrix components correspond to reflection and transmission amplitudes (the corresponding coefficients are ratios of particle fluxes). So, we write, instead of (2), the following functions:

$$\psi_L = A_1 \frac{e^{ikx}}{\sqrt{k}} + B_1 \frac{e^{-ikx}}{\sqrt{k}}, \quad x \rightarrow -\infty \quad (7)$$

$$\psi_R = A_2 \frac{e^{i\kappa x}}{\sqrt{\kappa}} + B_2 \frac{e^{-\kappa x}}{\sqrt{\kappa}}, \quad x \rightarrow \infty \quad (8)$$

In (7) and (8)  $k$  and  $\kappa$  coincide with the particle velocities at infinity because we put  $\hbar = m = 1$ . The functions  $\psi_L$  and  $\psi_R$  are asymptotes of one and the same exact solution. Hence, the following relations between coefficients  $A_i$  and  $B_i$  exist<sup>1</sup>:

$$A_2 = \alpha A_1 + \beta B_1, \quad B_2 = \beta^* A_1 + \alpha^* B_1 \quad (9)$$

Since the wave functions are now normalized to unit fluxes, the particle conservation law (or the continuity condition for the current) reads

$$|A_1|^2 - |B_1|^2 = |A_2|^2 - |B_2|^2 \quad (10)$$

Substituting here  $A_2$  and  $B_2$  from (9) leads to

$$|\alpha|^2 - |\beta|^2 = 1 \quad (11)$$

One has from (9):

$$A_1 = \frac{1}{\alpha} A_2 - \frac{\beta}{\alpha} B_1, \quad B_2 = \frac{\beta^*}{\alpha} A_2 + \frac{1}{\alpha} B_1 \quad (12)$$

This means, that the scattering matrix has the form:

$$\hat{S} = \begin{pmatrix} 1/\alpha & -\beta/\alpha \\ \beta^*/\alpha & 1/\alpha \end{pmatrix} \quad (13)$$

It is easy to check using (11), that this matrix is unitary. The reflection and transmission coefficients are respectively

$$R = |\beta/\alpha|^2 = |\beta/\alpha^*|^2, \quad T = |\alpha|^{-2}$$

and  $T + R = 1$  as it should be.

It is instructive to note in conclusion, that the problem of normalization does not appear in the typical 3-d situations where the scattering potential vanishes at infinity. Nevertheless it is helpful sometimes to use the normalization to unit flux as e.g. in the Born approximation (c.f. Ref. [1] § 126).

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<sup>1</sup> L.D. Landau and E.M. Lifshitz, *Quantum Mechanics*, Nauka, Moscow (1974)

<sup>2</sup> B.D. Kandilarov, V. Decheva, *J. Phys. C* **10** (1977) 1703

<sup>3</sup> B.D. Kandilarov, V. Decheva, *J. Phys. C* **11** (1978) L919

<sup>4</sup> V. Decheva, B.D. Kandilarov, *Surf. Science* **64** (1977) 785

<sup>5</sup> V. Decheva, B.D. Kandilarov, *Phys. Stat. Sol. B* **96** (1979) 877